Indian J. Phys. **78(10)**, 1085-1093 (2004)

AN INTERNATIONAL JOURNAL
IJP

Electron excitation of the *D* states of the alkaline earth atoms

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Abstract : We have used distorted wave (DW) approximation theory to study the excitation of the few lower excited $n^{1,3}D$ states of Ca (n = 4, 5) and Sr (n = 5, 6) from their ground state. Hartree-Fock wave functions obtained from Fischer's Code are used to represent the ground and excited states of the Ca and Sr atoms as well as to generate the distortion potentials for the projectile continuum electron distorted waves. Results for Stokes parameters are calculated at electron impact energies of 20 and 40 eV. Good agreement has been found on comparison with the relativistic distorted wave calculations.

Keywords : Distorted wave approximation, alkaline earth atom, excitation of *D* states.

PACS Nos. : 34.80.Dp, 34.80.Nz

1. Introduction

Most of the earlier studies on electron impact excitation of atoms have been confined on the *S-S* and *S-P* transitions. It is only recently that some groups have focused on studying the *S-D* excitations in some lighter atoms like hydrogen and helium. The excitation of the *D* states of atoms is of increasing interest [1] since carrying out 'perfect scattering experiment' is emphasized [2]. Calculation of these states is more challenging than for the excitation of a *P* state. Our group has previously carried out relativistic distorted wave (RDW) calculations for the excitation of the *D* states of magnesium [3,4], calcium and strontium [5]. In these calculations, both the bound electrons of the atom as well as projectile continuum electrons are described relativistically and are obtained through solving the Dirac equations. In the present paper, we perform non-relativistic distorted wave (DW) calculations for the Stokes parameters of the emitted photons while the excited $n^{1,3}D$ states of Ca (n = 4, 5) and Sr (n = 5, 6) decay to their lower *P* state. This *P* state may further subsequently decay by another cascading photon emission to a still lower *S* state. We present our DW results and compare with the RDW calculations at electron impact energies of 20 and 40 eV. The comparison thus provides the importance of relativistic effects. There are no experimental results at the moment to compare with these calculations, however, there are plans to measure the Stokes parameters for the excitation of these *D* states in the alkaline earth atoms (Crowe, private communication).

In the next Section 2, we present in brief the *T*-matrix in DW approximation theory and its connection with the Stokes parameters. In Section 3, results are presented and discussed.

2. Theoretical considerations

2.1. T-matrix in DW approximation :

In the present study, the alkaline earth atoms (namely Ca and Sr) are treated as two-electron systems and the effect of core electrons is incorporated in the form of a core potential. The transition matrix for the electron impact excitation of alkaline earth atoms from its initial state i to a final magnetic sub-state f_M in the distorted wave approximation (DW) can be written as

$$= \left\langle \chi^-_{f_M} \left| V - U_f \right| A\chi^+_i \right\rangle, \qquad (1)$$

where A is the antisymmetrization operator which takes into account the electron exchange effect between projectile and target electrons, V is the total interaction potential

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between the target alkaline earth atom and the projectile electron given by (atomic units are used throughout)

$$V = -\frac{z}{r_3} + \frac{1}{|r_2 - r_3|} + \frac{1}{|r_1 - r_3|} + V^{\text{core}}(r_3). \quad (2)$$

Here, r_1, r_2 and r_3 are respectively the position coordinates of the target valence electrons and the projectile electron with respect to the target nucleus. Further, the core potential, V^{core}, of the alkaline earth atom is given by

$$V^{\text{core}} = \sum_{n=1}^{j} N_{nl} \int \frac{|R_{nl}(r)|^2 r^2 dr}{} \quad (3)$$

where j = 3 and 4 respectively for Ca and Sr atoms, N_{nl} represents the occupation number of the electrons in different orbitals referred to by n and l quantum numbers and R_{nl} is the corresponding radial wave functions.

$\chi_i^+(\chi_{f_M}^-)$ is the combined wave function of the distorted wave projectile electron and target state of alkaline atoms in the initial (final) channel. It is defined as

$$\chi_{i(f_M)}^{+(-)} = F^{+(-)}(k_{i(f)}, r_3)\Psi_{i(f_M)}(r_1, r_2)\, S_{i(f)}(1,2,3), \quad (4)$$

where $\Psi_{i(f_M)}$ is the initial (final) state wave function of the target alkaline atom and $S_{i(f)}(1,2;3)$ is the initial (final) state spin function for the composite system consisting of the incident projectile and the target. $F_{i(f)}^{+(-)}$ represents the initial (final) channel projectile distorted wave with the wave vector $k_i(k_f)$ and the associated superscript +(–) indicates the usual outgoing (incoming) wave boundary condition. The distorted waves are the solution of

$$[\nabla_3^2 + k_{i(f)}^2 - 2U_{i(f)}(r_3)]F^{+(-)}(k_{i(f)}, r_3) = 0. \quad (5)$$

Here, $U_{i(f)}$ is the distorted potential in the initial (final) channel.

Further, on substituting the expressions for χ_i^+ and $\chi_{f_M}^-$ from eq. (4) into the expression of the T-matrix (eq. (1)), we get

$$T_{if_M} = \left\langle \begin{matrix} F^-(k_f, r_3)\Psi_{f_M}(r_1, r_2)\, S_f(1,2;3)\left|V - U_f\right| \\ F^+(k_i, r_3)\Psi_i(r_1, r_2)\, S_i(1,2;3) \end{matrix} \right\rangle$$

$$- \left\langle \begin{matrix} F^-(k_f, r_3)\Psi_{f_M}(r_1, r_2)\, S_f(1,2;3)\left|V - U_f\right| \\ F^+(k_i, r_1)\Psi_i(r_3, r_2)\, S_i(3,2;1) \end{matrix} \right\rangle. \quad (6)$$

Further, the scattering amplitude a_M in the 'collision frame of reference' for the electron impact excitation of the atom from an initial state i to a final magnetic substate f_M is related to the DW transition matrix elemen T_{if_M} by

$$a_M = -\frac{1}{2\pi} T_{if_M}. \quad (7$$

The expression for the T-matrix eq. (6) can be simplifie further for a specific transition by carrying out th integration over the spin coordinates. In this paper, w consider two types of transitions : (i) the excitation fro the ground $n\ ^1S$ state to excited $n'\ ^1D$ *i.e.* singlet t singlet (SS) transition and (ii) the excitation from th ground state $n\ ^1S$ state to $n'\ ^3D$ states *i.e.* singlet to triplc (ST) excitations in Ca (n = 4, n' = 4, 5) and Sr (n = 5 n' = 5, 6). We give here a brief outline how to evaluat the T-matrix for each SS and ST excitation processes.

Singlet-singlet excitations ($n\ ^1S$-$n'\ ^1D$)

In the singlet-singlet excitations the scattering takes plac in the doublet mode *i.e.* the total spin of the system S 1/2. The doublet mode spin function S_i (S_f) in terms o the usual Dirac matrices α and β for the composit system is given by [6]

$$S_{i(f)}(1,2;3) = \frac{1}{\sqrt{2}}\alpha_3(\alpha_1\beta_2 - \alpha_2\beta_1). \quad (8$$

Substituting $S_{i(f)}$ in eq. (6) and carrying out the spi integration using the orthogonal properties of individua spin functions *i.e.*

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij},$$

$$\beta_i | \beta_j \rangle = \delta_{ij},$$

$$\alpha_i | \beta_j \rangle = 0, \quad (9$$

we get

$$T_{if_M} = T_{if_M}^{\text{d}} - T_{if_M}^{\text{ex}} \quad (10$$

In eq. (10), $T_{if_M}^{\text{d}}$ and $T_{if_M}^{\text{ex}}$ are the spin averaged direc and exchange T-matrices expressed as

$$T_{if_M}^{\text{d}} = \int F^{-*}(k_f, r_3)\Psi_{f_M}^*(r_1, r_2)(V - U_f(r_3))F^+ (k_i, r_3)\Psi_i(r_1, r_2)dr_1 dr_2 dr_3, \quad (11$$

$$T_{if_M}^{\text{d}} = \int F^{-*}(k_f, r_3)\Psi_{f_M}^*(r_1, r_2)(V - U_f(r_3)) F^+(k_i, r_1)\Psi_i(r_3, r_2)dr_1 dr_2 dr_3.$$

Singlet-triplet excitations (n ^{1}S-n' ^{3}D)

In the singlet-triplet excitations, the scattering takes place in the doublet mode, *i.e.* in this mode also the total spin of the composite system $S = 1/2$. This is because of the conservation of the total spin of the system during the excitation process. The expressions for S_i and S_f in the ST excitation are given by

$$S_i = \frac{1}{\sqrt{2}}\alpha_3[\alpha_1\beta_2 - \alpha_2\beta_1], \tag{13}$$

$$S_f = \frac{1}{\sqrt{6}}[2\alpha_1\alpha_2\beta_3 - \alpha_3(\alpha_1\beta_2 + \alpha_2\beta_1)]. \tag{14}$$

On substituting these in the T-matrix eq. (6) and carrying out the spin integrations we get

$$T_{if_M} = \sqrt{3}T^{ex}_{if_M}. \tag{15}$$

Here, the direct transition matrix $T^d_{if_M}$ does not appear because the ST excitation cannot take place without an interchange of the projectile and target electron.

Choice of distortion potential and wave functions

For the calculation of the distorted waves using eq. (5), the distortion potential $U_{i(f)}$ is taken as the sum of the spherical average of static potential and exchange distortion potential *i.e.*

$$U_{i(f)} = V^{stat}_a + V^{ex}_{i(f)} \quad \text{(with a = i or f)}. \tag{16}$$

Here, $V^{stat}_a = \langle\phi_a|V|\phi_a\rangle$ is the spherically averaged static potential of the alkaline earth atom in the initial ($a = i$) or final ($a = f$) state and is given by

$$V^{stat}_a(r_3) = -\frac{2}{r_3} + V^{core}(r_3) + 2\int_0^\infty \frac{|R_a(r_1)|^2}{\max(r_1, r_3)} r_1^2 dr_1$$

(with $a = i$ or f). (17)

$V^{exch}_{i(f)}$ is the exchange distortion potential in the initial (final) channel and is taken for the work of Furness and McCarthy [7].

$$V^{exch}_{i(f)}(r_3) = \frac{1}{2}\left\{\left(\frac{1}{2}k^2_{i(f)} - V^{stat}_a(r_3)\right) - \left[\left(\frac{1}{2}k^2_{i(f)} - V^{stat}_a(r_3)\right)^2 - 8\pi\tau\rho_a(r_3)\right]\right\}. \tag{18}$$

Here, $\rho_a(r) = \int|\phi_a(r, r')|^2 dr'$ is the spherical average of the one electron charge density of the alkaline atom in the initial or final channel. The value of the parameter τ depends on the total spin of the colliding system and is taken from the paper of Vucic *et al* [8]. For example, in case of the excitation of Ca atom, for the channel e–Ca (n^3L) $\tau = -1$ and for the channel e + Ca (n^1L), $\tau = 1$. To obtain V^{stat}_a and ρ_a, we use the same target wave functions as for the evaluation of the T-matrix.

In order to evaluate integrals [eqs. (11) and (12)], we require the wave functions for Ca and Sr atoms in their initial and final states. For this purpose the Hartree-Fock wave functions have been used which are obtained from the Fischer's computer code [9].

2.2. Stokes parameters P_i (i = 1–4) :

The differential Stokes parameters P_i (i = 1–3) for the photon emitted after the excitation of atoms by electrons, measured perpendicular to the scattering plane are :

$$P_1 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)}, \tag{19}$$

$$P_2 = \frac{I(45°) - I(135°)}{I(45°) + I(135°)}, \tag{20}$$

$$P_3 = \frac{I(\text{RHC}) - I(\text{LHC})}{I(\text{RHC}) + I(\text{LHC})}. \tag{21}$$

While, analogous to P_1, the Stokes parameter P_4 measured parallel to the scattering plane is given by

$$P_4 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)}, \tag{22}$$

where $I(\phi)$ is the intensity of light with polarization detector in the ϕ direction with respect to incident electron direction and I (RHC) and I (LHC) are respectively the intensities of the right and left circularly polarized light components, respectively.

Blum [10] gave explicit expressions for the Stokes intensities in terms of the state multipoles $\langle T(L)^+_{KQ}\rangle$ for the photons emitted in direction $(\theta_\gamma, \phi_\gamma)$ in coincidence with the scattered electrons after impact excitation of an atomic state with orbital angular momentum L and an electric dipole transition to a state with orbital angular momentum L_2 in the 'collision frame of reference'. Thus, the Stokes parameters P_i(i = 1,2,3 and 4) for any $L \rightarrow L_2$ decay may be given by

$$P_1 = \frac{1}{I^\gamma}\begin{Vmatrix} 1 & 1 & \\ L & L & L_2 \end{Vmatrix} \cdot \sqrt{\frac{3}{2}}G_2(L)\langle T(L)^+_{20}\rangle - G_2(L)\langle T(L)^+_{22}\rangle \tag{23}$$

$$P_2 = \frac{1}{I^y}\begin{Bmatrix}1 & 1 & 2\\ L & L & L_2\end{Bmatrix}\left[2G_2(L)\left\langle T(L)^+_{21}\right\rangle\right], \tag{24}$$

$$P_3 = \frac{1}{I^y}\begin{Bmatrix}1 & 1 & 1\\ L & L & L_2\end{Bmatrix}\left[2iG_1(L)\left\langle T(L)^+_{11}\right\rangle\right], \tag{25}$$

$$P_4 = \frac{1}{I^x}\begin{Bmatrix}1 & 1 & 2\\ L & L & L_2\end{Bmatrix} \left[\frac{3}{2}G_2(L)\left\langle T(L)^+_{20}\right\rangle + G_2(L)\left\langle T(L)^+_{22}\right\rangle\right] \tag{26}$$

where

$$= \frac{2(-1)^{L+L_2}}{3(2L+1)^{1/2}}G_0(L)\left\langle T(L)^+_{00}\right\rangle + \begin{Bmatrix}1 & 1 & 2\\ L & L & L_2\end{Bmatrix} \left[\frac{G_2(L)}{\sqrt{6}}\left\langle T(L)^+_{20}\right\rangle + G_2(L)\left\langle T(L)^+_{22}\right\rangle\right] \tag{27}$$

and

$$I^x = \frac{2(-1)^{L+L_2}}{3(2L+1)^{1/2}}G_0(L)\left\langle T(L)^+_{00}\right\rangle + \begin{Bmatrix}1 & 1 & 2\\ L & L & L_2\end{Bmatrix} \left[\frac{G_2(L)}{\sqrt{6}}\left\langle T(L)^+_{20}\right\rangle - G_2(L)\left\langle T(L)^+_{22}\right\rangle\right]. \tag{28}$$

$G_K(L)$ are the depolarization perturbation coefficients which account for the fine structure of the final excited state and are given by

$$G_K(L) = \frac{1}{(2S+1)}\sum_J (2J+1)^2\begin{Bmatrix}L & J & S\\ J & L & K\end{Bmatrix}^2, \tag{29}$$

where S is the electron spin and $J = L + S$ is the total angular momentum of the atom. The $G_K(L)$ are normalized such that $G_0(L) = 1$ for all L.

Further, $\left\langle T(L)^+_{KQ}\right\rangle$ are the state multipoles of the excited state with orbital angular momentum L. These state multipoles are related to the complex scattering amplitudes as

$$\left\langle T(L)^+_{KQ}\right\rangle = \sum_{M',M}(-1)^{L-M'}(2K+1)^{1/2}\begin{pmatrix}L & L & K\\ M' & -M & -Q\end{pmatrix} \left\langle a(M')a(M)^*\right\rangle, \tag{30}$$

where

$$\left\langle a(M')a(M)^*\right\rangle \frac{}{2(2S_i+1)} \sum(2S+1)a(M')^S a(M)^{S*}. \tag{31}$$

Here, $a(M)^S$ is the scattering amplitude for excitation of the magnetic substate M in the channel with total spin S and S_i is the spin of the initial target state. From the properties of the $3j$ symbol, the values of K and component Q of the multipoles are restricted by the condition $K \le 2L$ and $-Q \le K \le Q$.

The state multipole $\left\langle T(L)^+_{00}\right\rangle$ is a measure of the overall population of the atomic state and can be expressed in terms of the differential cross section σ as

$$\left\langle T(L)^+_{00}\right\rangle = \frac{\sigma}{(2L+1)^{1/2}}. \tag{32}$$

Further, we see from eq. (25) that $\left\langle T(L)^+_{1Q}\right\rangle$ describes the orientation of the state and thus the circular polarization of the emitted photons. The state multipole $\left\langle T(L)^+_{2Q}\right.$ describes the alignment of the atomic state and thus gives the anisotropic part of the coincidence rate and the linear polarization of the emitted photon. Also note that for dipole transitions it is impossible to achieve state multipoles with rank $K > 2$ since a single photon has an angular momentum of unity.

The excited $n\ ^1D$ and $n\ ^3D$ states after excitation decay by dipole transition, photons to the lower P states *i.e.* $n\ ^1P$ and $n\ ^3P$ states. Therefore taking $L = 2$, $L_2 = 1$ in eqs. (23–28), the Stokes parameter for a $^{1,3}D \rightarrow {}^{1,3}P$ de-excitation process can be expressed in terms of state multipoles $\left\langle T(D)^+_{KQ}\right\rangle$ as

$$P_1 = \frac{1}{I^y}\frac{1}{10}\sqrt{\frac{7}{3}}\left[\sqrt{\frac{3}{2}}\left\langle T(D)^+_{20}\right\rangle - G_2\left\langle T(D)^+_{22}\right\rangle\right. \tag{33}$$

$$P_2 = \frac{-1}{I^y}\frac{1}{10}\sqrt{\frac{7}{3}}\left[2G_2\left\langle T(D)^+_{21}\right\rangle\right], \tag{34}$$

$$P_3 = \frac{-1}{I^y}\frac{1}{\sqrt{5}}\left[iG_1\left\langle T(D)^+_{11}\right\rangle\right], \tag{35}$$

$$P_4 = \frac{1}{I^x}\frac{1}{10}\sqrt{\frac{7}{3}}\left[\sqrt{\frac{3}{2}}G_2\left\langle T(D)^+_{20}\right\rangle + G_2\left\langle T(D)^+_{22}\right\rangle\right] \tag{36}$$

where

$$I^y = \frac{-2}{3\sqrt{5}}G_0\left\langle T(D)^+_{00}\right\rangle + \frac{1}{10}\times \sqrt{\frac{7}{3}}\left[\frac{G_2}{\sqrt{6}}\left\langle T(D)^+_{20}\right\rangle + G_2\left\langle T(D)^+_{22}\right\rangle\right] \tag{37}$$

$$I^x = \frac{-2}{3\sqrt{5}}G_0\left\langle T(D)^+_{00}\right\rangle + \frac{1}{10}\times \sqrt{\frac{7}{3}}\left[\frac{G_2}{\sqrt{6}}\left\langle T(D)^+_{20}\right\rangle - G_2\left\langle T(D)^+_{22}\right\rangle\right], \tag{38}$$

3. Results and discussion

We consider here the calculations of the Stokes parameters for Ca and Sr from the emitted photons while their excited $n\ ^{1,3}D$ states of Ca (n = 4, 5) and Sr (n = 5, 6) decay to their lower $^{1,3}P$ states. These P states may further subsequently decay by another cascading photon emission to a still lower S state.

In Figures 1 and 2, we have presented our DW results

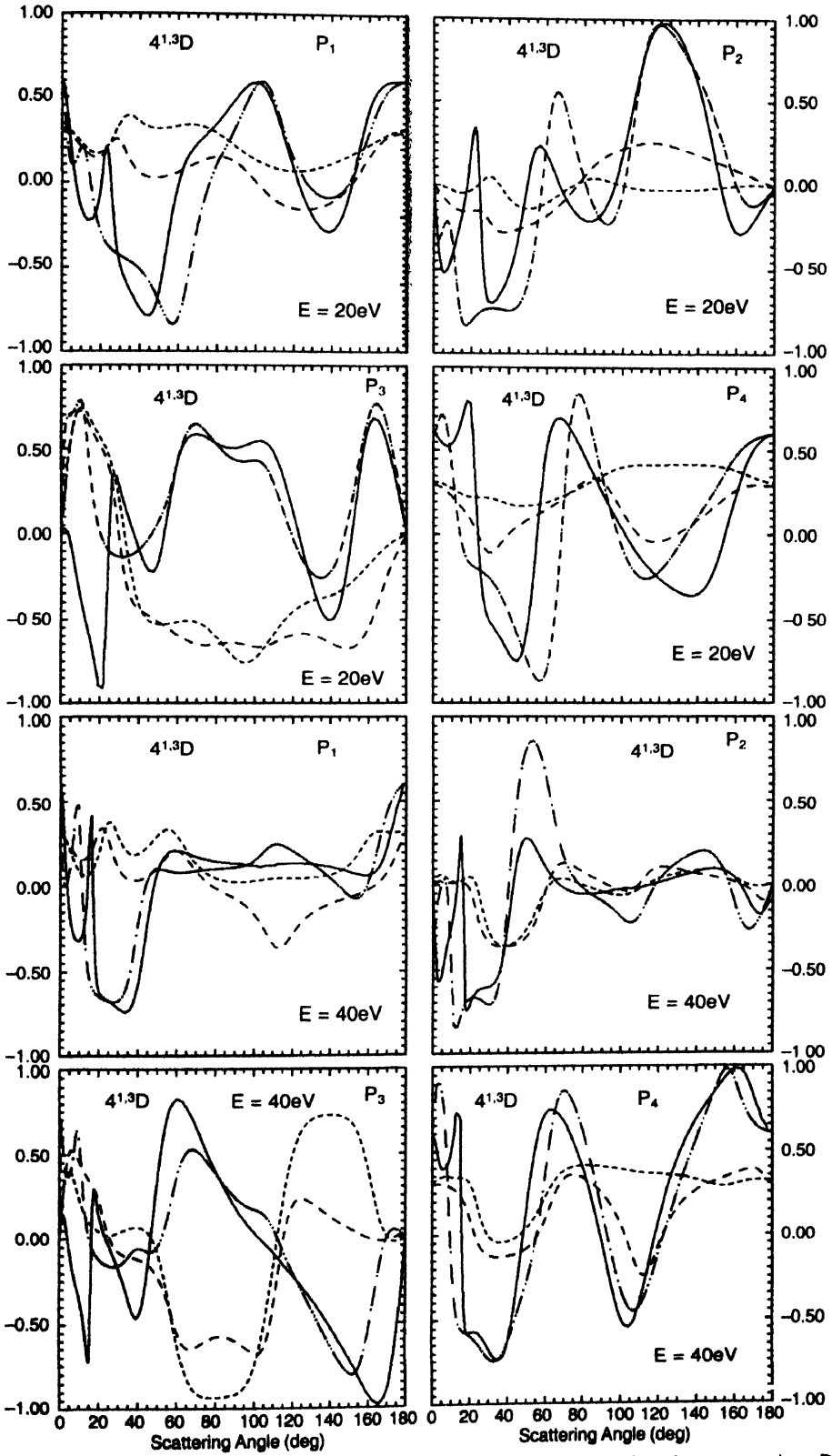

Figure 1. Stokes parameters P_1, P_2, P_3, P_4 for the excitation of the $4\ ^{1,3}D$ state of Ca at 20 and 40 eV incident electron energies—. DW results of $4\ ^1D$; RDW results of $4\ ^1D$; - - - - DW results of $4\ ^3D$; – – – – RDW results of $4\ ^3D$.

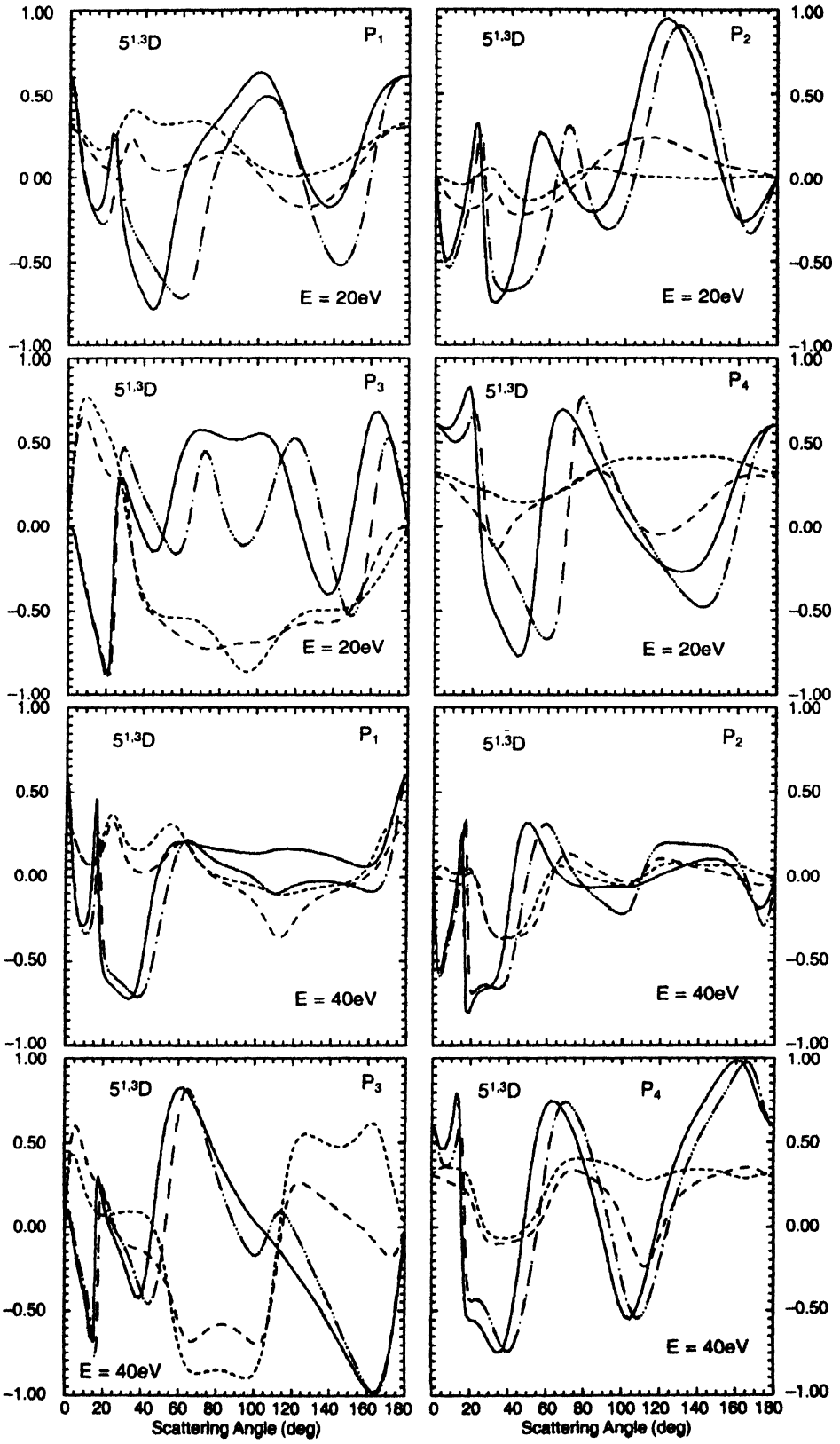

Figure 2. Stokes parameters P_1, P_2, P_3, P_4 for the excitation of the 5 $^{1,3}D$ state of Ca at 20 and 40 eV incident electron energies–. DW results of 5 ^1D; — — RDW results of 5 ^1D; ---- DW results of 5 ^3D; - - - - RDW results of 5 ^3D.

of the Stokes parameters P_1, P_2, P_3, P_4 respectively for the excitation of 4 $^{1,3}D$ and 5 $^{1,3}D$ states of calcium atom. These results are compared with the only available RDW calculations. We find that for both the 4 ^1D and 5 ^1D excitations, the DW and RDW calculations agree qualitatively and quantitatively in reasonable manner at

20 eV and in much better way at 40 eV. For the 4 ^3D and 5 ^3D excitations, the quantitative agreement of the two calculations is not so good. As expected, this may be due to the relativistic effect *i.e.* spin exchange and spin-orbit interactions which are incorporated in RDW calculations in a consistent manner. Comparing the results for $n = 4$ and 5 states of Ca, we notice that the structures shown are quite different. It is interesting to note that the Stokes parameters P_3 for both the triplet and singlet D excitations at 20 and 40 eV have the reverse nature in the RDW and DW calculations in the range of forward scattering. Consequently, the RDW calculations suggest violation of the propensity rule while DW calculations obey it and behave in normal manner. This is again due to the effect of relativistic contribution which need to be verified by future experiments. Similarly, Figures 3 and 4

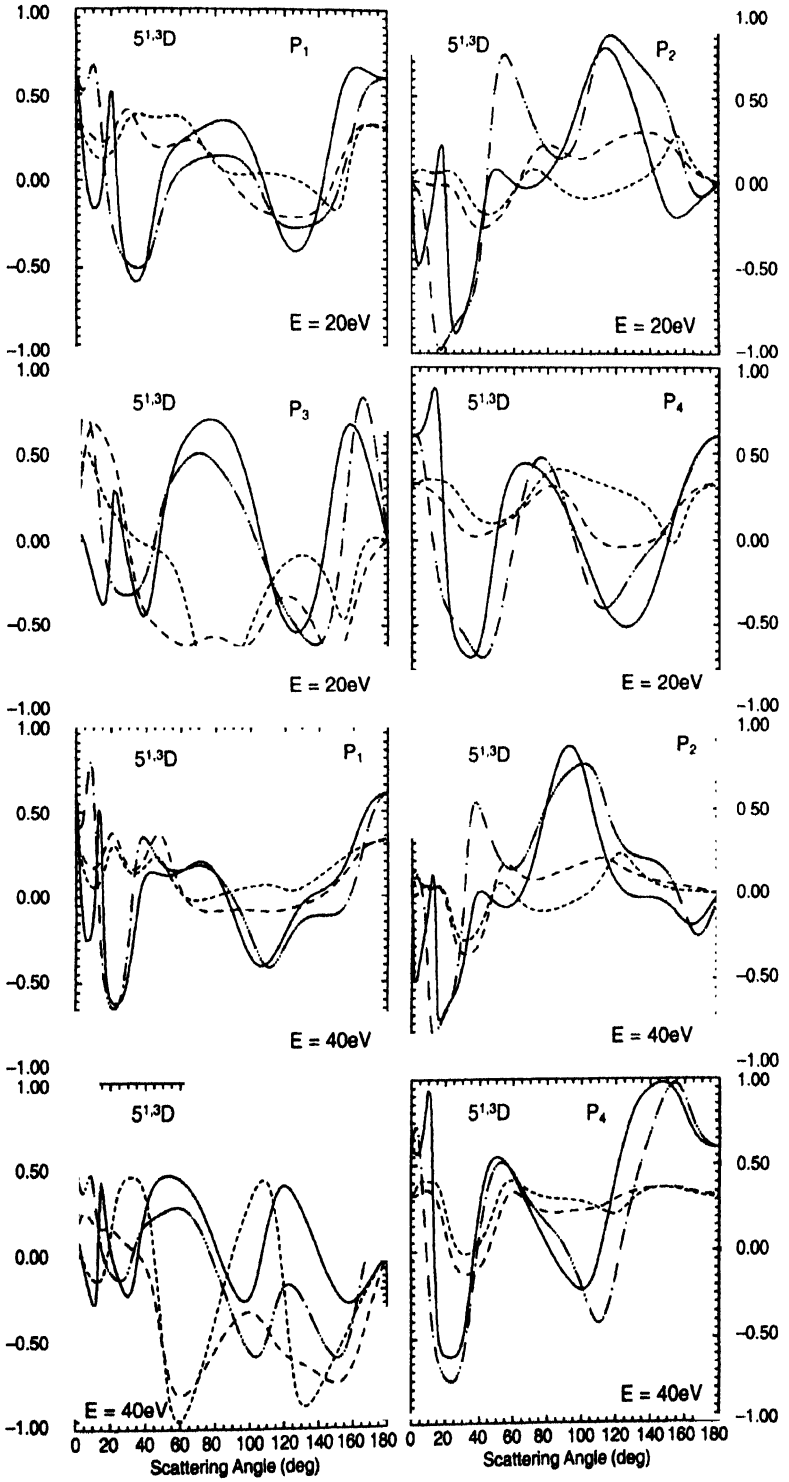

Figure 3. Same as in Figure 1 but for the excitation of the 5 $^{1,3}D$ state of Sr atom.

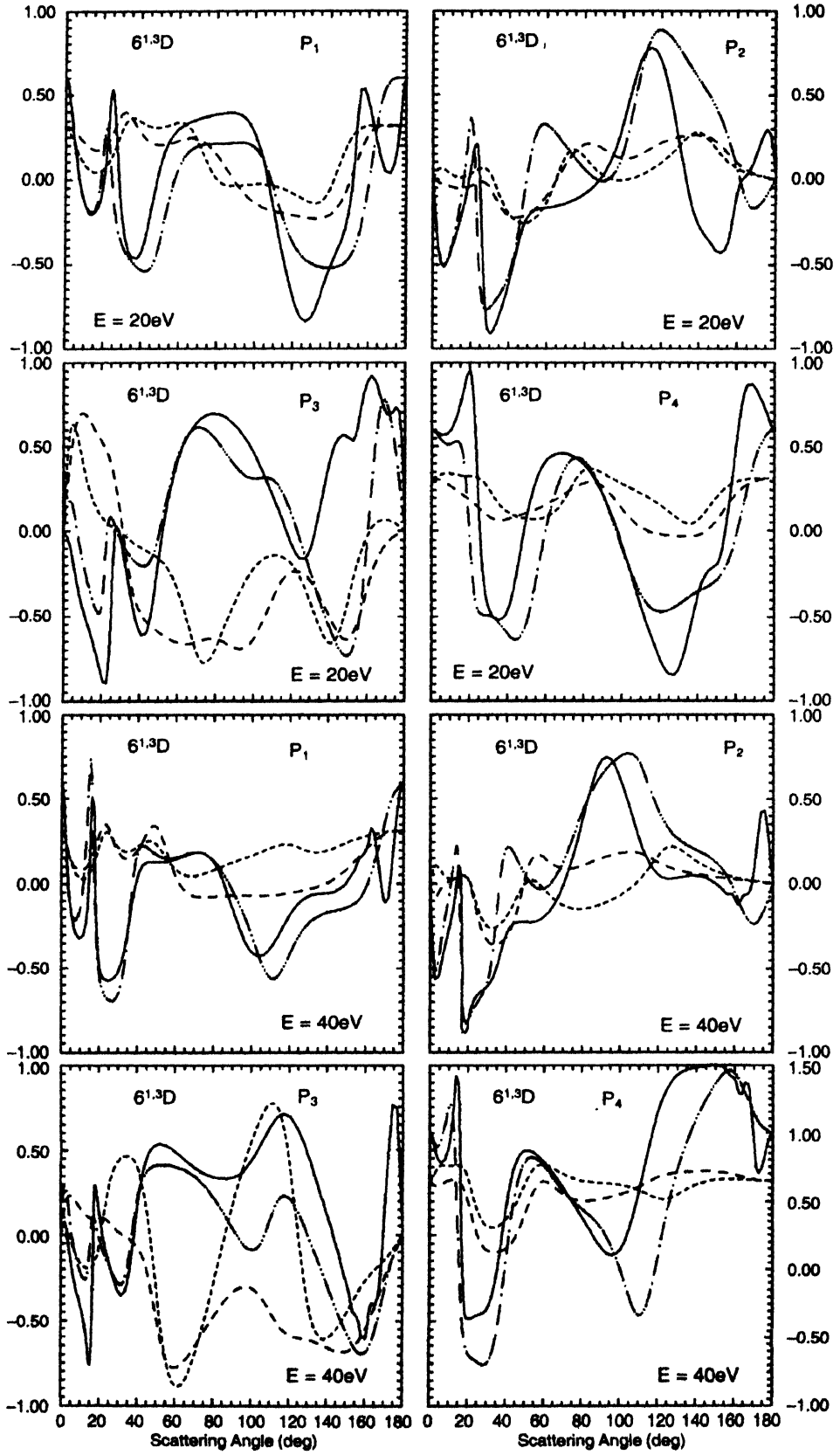

Figure 4. Same as in Figure 2 but for the excitation of the 6 $^{1,3}D$ state of Sr atom.

present the Stokes parameters for the excitation of 5 $^{1,3}D$ and 6 $^{1,3}D$ states of strontium atom. In these figures also, behaviour of the results is somewhat similar to that of calcium as presented in the Figures 1 and 2.

4. Conclusion

We have reported Stokes parameters for the excitation of the lower lying D states of the Ca and Sr at 20 and 40 eV. A reasonable agreement is found between the results predicted by the DW and RDW theories. The contribution of relativistic effects is also discussed in the results. We believe that our present results would be helpful in guiding the future experimental measurements and more theoretical calculations.

Acknowledgmnts

We are thankful to Prof. A D Stauffer for fruitful discussions. The financial assistance from the CSIR, New Delhi is gratefully acknowledged. One of us (SS) is thankful to CSIR for the Senior research fellowship.

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